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2D/3D Discrete Duality Finite Volume Scheme (DDFV) applied to ECG simulation.

DDFV scheme for anisotropic- heterogeneous elliptic equations, application to a bio-mathematics problem : electrocardiogram simulation.

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RÉSUMÉ.

ABSTRACT. In this paper is presented a finite volume (DDFV) scheme for solving elliptic equations with heterogeneous anisotropic conductivity tensor. That method is based on the definition of a discrete divergence and a discrete gradient operator. These discrete operators have close relationships with the continuous ones, in particular they fulfil a duality property related with the Green formula. The operators are defined in dimension 2 and 3, their duality property is stated and used to establish the well posedness of the approximation scheme as well as its symmetry/positiveness. In the last part, the method is used for the resolution of a problem arising in bio-mathematics: the ECG (electrocardiogram) simulation. This is done on a 2D slice of a realistic torso defined from segmented MRI medical images.

MOTS-CLÉS :

KEYWORDS: keywords

1. Introduction

The aim of this paper is to define a finite volume discretisation (called *DDFV* discretisation) for the following elliptic equation on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. For a conductivity tensor $G = G(x)$ (symmetric positive definite and uniformly elliptic on Ω) that is anisotropic and also heterogeneous, and for a mixed Neumann/Dirichlet homogeneous boundary condition on $\partial\Omega = \partial\Omega^N \cup \partial\Omega^D$, we search φ such that (\mathbf{n} is a unit normal on the boundary) :

$$\operatorname{div}(G\nabla\varphi) = f, \quad G\nabla\varphi \cdot \mathbf{n} = 0 \text{ on } \partial\Omega^N, \quad \varphi|_{\partial\Omega} = 0 \text{ on } \partial\Omega^D, \quad f \in L^2(\Omega). \quad (1)$$

Precisely, one assumes that there exists one (or more) crack Γ in the domain that splits Ω in Ω_1, Ω_2 and such that G has a discontinuity across Γ . One thus imposes the transmission condition (\mathbf{n} is a normal to Γ), in the trace sense on Γ :

$$\varphi|_{\Omega_1} = \varphi|_{\Omega_2}, \quad G|_{\Omega_1} \nabla\varphi|_{\Omega_1} \cdot \mathbf{n} = G|_{\Omega_2} \nabla\varphi|_{\Omega_2} \cdot \mathbf{n} \quad \text{on } \Gamma. \quad (2)$$

When $G|_{\Omega_i}$ is smooth enough, the classical theory (see *e.g.* [LAD 68]) tells us that (1) has a unique variational solution $\varphi \in H^1(\Omega)$ such that $\varphi|_{\Omega_i} \in H^2(\Omega_i)$ and such that the boundary condition in (1) and the transmission conditions in (2) hold in the trace sense. Whenever $\partial\Omega^N = \partial\Omega$, uniqueness doesn't hold anymore and there is then a solution iff f has zero mean value, all solution then differ up to a constant.

2. DDFV discretisation of the problem

2.1. Mesh definition and discrete data

We consider a Delaunay triangulation/tetrahedrisation \mathcal{C} of a bounded polygonal/polyhedral subset $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. We denote by \mathcal{V} and \mathcal{I} the associated sets of vertices and interfaces (elements edges/faces). The elements $C \in \mathcal{C}$ will be called *primal cells*. For equation (1) to be correctly discretised, we naturally assume that the internal interfaces "follow" cracks in G and that the boundary interfaces $\sigma \subset \partial\Omega$ are dealt into two subsets $\mathcal{I}^D, \mathcal{I}^N$ such that $\Omega^N = \cup_{\sigma \in \mathcal{I}^N} \sigma$, $\Omega^D = \cup_{\sigma \in \mathcal{I}^D} \sigma$. The set of vertices of the interfaces $\sigma \in \mathcal{I}^D$ is denoted by $\mathcal{V}^D \subset \mathcal{V}$.

To every primal cell C is associated a centre $K \in C$ (its iso-barycentre in practice). By C_K one denotes the primal cell C of centre K . To any interface $\sigma \in \mathcal{I}$ is associated a centre $Y_\sigma \in \sigma$ (also its iso-barycentre in practice), also simply denoted Y . Every internal interface $\sigma \in \mathcal{I}$ is the boundary between two primal cells C_1 and C_2 . This is denoted by $\sigma = C_1|C_2$. For more simplicity one shall denote by the same symbol any geometrical element and its measure : if $\sigma \in \mathcal{I}$, σ also denotes its length/area ; if $C \in \mathcal{C}$, C also denotes its area/volume, Ω both denotes the domain and its measure...

To every vertex $A \in \mathcal{V}$ is associated a **dual cell** P_A . Let us first introduce the subset $\mathcal{I}_A \subset \mathcal{I}$ of all the interfaces having A as a vertex. To every $\sigma \in \mathcal{I}_A$ is associated a geometrical element $P_{A,\sigma}$. P_A is given by $P_A = \cup_{\sigma \in \mathcal{I}_A} P_{A,\sigma}$.

The elements $P_{A,\sigma}$ are defined as follows (see figure 2.1). Let $\sigma = C_{K_1}|C_{K_2}$ be an

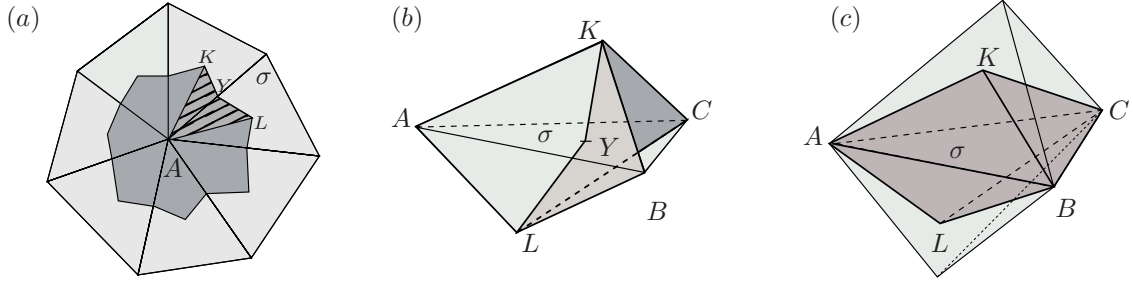


Figure 1. (a) Two dimensional case, definition of $P_{A,\sigma}$ (hatched dark grey) and P_A (dark grey). (b) Three dimensional case, definition of $P_{A,\sigma}$ for an internal interface $\sigma = C_K|C_L = ABC$. (c) Three dimensional diamond cell D_σ (dark grey). $D_\sigma = D_{\sigma,K} \cup D_{\sigma,L}$, $D_{\sigma,K}$ is the part above σ whereas $D_{\sigma,L}$ is the part underneath σ .

internal interface and let Y be σ 's centre. In dimension 2, $P_{A,\sigma}$ is the quadrilateral AK_1YK_2 . In dimension 3, let B and C be the two other vertices of σ ($\sigma = ABC$). Then $P_{A,\sigma}$ is the reunion of the two pyramids having the same quadrilateral base $ABYC$ and K_1, K_2 for apex : $P_{A,\sigma} = ABYCK_1 \cup ABYCK_2$. That definition has obvious extension to the case $\sigma \subset \partial\Omega$.

Remark that in dimension 2 the (interiors of the) dual cells are disjoint and recover the whole domain, therefore $\sum_{A \in \mathcal{V}} P_A = \Omega$. Whereas in dimension 3 the dual cells are no more disjoint, if A and B are two vertices of the same interface σ , $P_{A,\sigma} \cap P_{B,\sigma} \neq \emptyset$. Actually the dual cells now recover exactly twice the whole domain, so that $\sum_{A \in \mathcal{V}} P_A = 2\Omega$.

To every interface $\sigma \in \mathcal{I}$ is associated one **diamond cell** D_σ . For an internal interface $\sigma = C_K|C_L$, it is defined as $D_\sigma = D_{\sigma,K} \cup D_{\sigma,L}$ where $D_{\sigma,K}, D_{\sigma,L}$ are the two triangles/pyramids with base σ and apex K and L respectively, as depicted on figure 2.1. In the case of a boundary interface $\sigma \subset \partial\Omega$, D_σ is a simple triangle/pyramid, $D_\sigma = D_{\sigma,K}$. The $D_{\sigma,K}$ will be called sub-diamond cells.

To this different types of cells are associated the following types of data :

A **discrete vector field** \mathbf{X}_h (resp. **discrete tensor** G_h) is a vector (resp. matrix) function, piecewise constant on each sub-diamond cell $D_{\sigma,K}$. To each internal interface $\sigma = C_K|C_L$ are associated two vectors $\mathbf{X}_{\sigma,K}$ and $\mathbf{X}_{\sigma,L}$ (resp. matrices $G_{\sigma,K}$ and $G_{\sigma,L}$) on each side of σ . $G_{\sigma,K}$ is always assumed symmetric positive definite. We shall say that \mathbf{X}_h is conservative relatively to G_h if (\mathbf{n}_σ being a normal to σ) :

$$\forall \sigma \in \mathcal{I} \text{ such that } \sigma = C_K|C_L : G_{\sigma,K} \mathbf{X}_{\sigma,K} \cdot \mathbf{n}_\sigma = G_{\sigma,L} \mathbf{X}_{\sigma,L} \cdot \mathbf{n}_\sigma, \quad (3)$$

A **discrete scalar** φ_h is the data of two sets of scalars $(\varphi_A)_{A \in \mathcal{V}}, (\varphi_K)_{K \in \mathcal{C}}$ associated to the vertices and primal cells centres respectively.

A **DDFV function** is a scalar function $\tilde{\varphi}_h$, piecewise affine on $AY_\sigma K$ (resp. $ABY_\sigma K$) whenever $\sigma \in \mathcal{I}$, $A \in \mathcal{V}$ (resp. $A, B \in \mathcal{V}$) is (are) vertex(es) of σ in dimension 2 (resp. 3) and $\sigma \subset C_K, C_K \in \mathcal{C}$.

2.2. The discrete operators and the problem discretisation

The **discrete divergence** div_h of a discrete vector field \mathbf{X}_h is the discrete scalar :

$$(\text{div}_h \mathbf{X}_h)_A = \frac{1}{P_A} \int_{\partial P_A} \mathbf{X}_h \cdot \mathbf{n}_{\partial P_A} ds, \quad (\text{div}_h \mathbf{X}_h)_K = \frac{1}{C_K} \int_{\partial C_K} \mathbf{X}_h \cdot \mathbf{n}_{\partial C_K} ds, \quad (4)$$

where $\mathbf{n}_{\partial E}$ is the outward unit normal on the boundary of the polygonal/polyhedral element E. That definition makes sense because there are no discontinuities of \mathbf{X}_h on the edges/faces of primal and dual cells.

The **discrete gradient** of a DDFV function $\tilde{\varphi}_h$ is the discrete vector field :

$$(\nabla_h \tilde{\varphi}_h)_{\sigma,K} = \frac{1}{D_{\sigma,K}} \int_{D_{\sigma,K}} \nabla \varphi_h dx. \quad (5)$$

The discrete gradient for a discrete scalar is defined below, for implementation, a practical formulation is given in appendix A.

Definition 2.1. Let us consider a discrete scalar φ_h such that $\varphi_A = 0$ for all $A \in \mathcal{V}^D$ and a discrete tensor G_h . Then there exists a unique DDFV function $\tilde{\varphi}_h$ such that :

$$\begin{aligned} \forall A \in \mathcal{V} : \tilde{\varphi}_h(A) &= \varphi_A, \quad \forall C_K \in \mathcal{C} : \tilde{\varphi}_h(K) = \varphi_K, \\ \forall \sigma \in \mathcal{I}^D : \tilde{\varphi}_h(Y_\sigma) &= 0, \quad \forall \sigma \in \mathcal{I}^N : G_\sigma (\nabla_h \tilde{\varphi}_h)_\sigma \cdot \mathbf{n}_\sigma = 0, \end{aligned}$$

and such that $\nabla_h \tilde{\varphi}_h$ is conservative relatively to G_h , as defined in (3).

Relatively to G_h , the discrete gradient of φ_h is defined as $\nabla_h \varphi_h = \nabla_h \tilde{\varphi}_h$.

The previously defined discrete operators fulfil a duality property called **discrete Green formula** by analogy with the continuous case :

Proposition 2.2. Let G_h a discrete tensor, φ_h a discrete scalar and consider the DDFV function $\tilde{\varphi}_h$ associated to φ_h relatively to G_h . If \mathbf{X}_h is a discrete vector field that satisfy $\mathbf{X}_{\sigma,K} \cdot \mathbf{n}_\sigma = \mathbf{X}_{\sigma,L} \cdot \mathbf{n}_\sigma$ on every internal interface $\sigma = C_K|C_L$, then :

$$\begin{aligned} \int_{\Omega} (\nabla_h \varphi_h) \cdot \mathbf{X}_h dx &= -\frac{1}{d} \sum_{C_K \in \mathcal{C}} \varphi_K (\text{div}_h \mathbf{X}_h)_K C_K - \frac{d-1}{d} \sum_{A \in \mathcal{V}} \varphi_A (\text{div}_h \mathbf{X}_h)_A P_A \\ &\quad + \int_{\partial \Omega} \tilde{\varphi}_h|_{\partial \Omega} \mathbf{X}_h|_{\partial \Omega} \cdot \mathbf{n}_{\partial \Omega} ds \end{aligned} \quad (6)$$

The consequence is the following :

Proposition 2.3. The right hand side f in (1) being discretised in some discrete scalar f_h , we look for a discrete scalar φ_h such that :

$$\begin{aligned} \forall A \in \mathcal{V}^D : \varphi_A &= 0, \quad \forall \sigma \in \mathcal{I}^N : G_\sigma (\nabla_h \varphi_h)_\sigma \cdot \mathbf{n}_\sigma = 0, \\ \forall A \in \mathcal{V} - \mathcal{V}^D : (\text{div}_h (G_h \nabla_h \varphi_h))_A &= f_A, \quad \forall C_K \in \mathcal{C} : (\text{div}_h (G_h \nabla_h \varphi_h))_K = f_K \end{aligned} \quad (7)$$

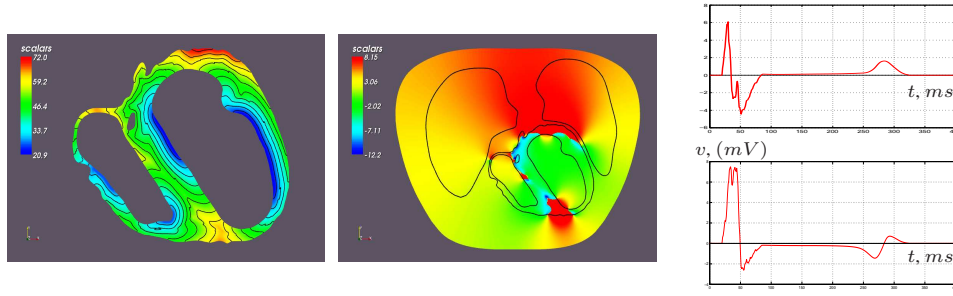


Figure 2. (left) Simulation of v : isochrons (ms) for the excitation wave on a 2D ventricles slice mesh coming from MRI segmented images, 485000 degrees of freedom. (middle) Computation of φ at time $t = 50\text{ms}$. The four domain are separated with black lines (ventricles, ventricles cavities, lungs and torso remaining). (right) Simulated ECG for two leads (V1 and V2) located on the body surface.

Such a φ_h satisfies the transmission conditions (2) in a discrete sense by construction. If $\mathcal{I}^D \neq \emptyset$, (7) has a unique solution. The resulting numerical linear problem to invert is moreover symmetric positive definite. The Neumann problem ($\mathcal{I}^D = \emptyset$) has a solution iff $\frac{1}{d} \sum_{C_K \in \mathcal{C}} f_K C_K + \frac{d-1}{d} \sum_{A \in \mathcal{V}} f_A P_A = 0$. The linear problem to invert is now symmetric positive, its kernel is composed of the discrete scalar ψ_h such that $\psi_A = C_1$, $\psi_K = C_2$.

3. Application

The bidomain model (see e.g. [KEE 98]) describes the electrical activity of the heart. It involves two compartments : the intra/extra cellular mediums, and models a trans-membrane potential $v = \varphi_i - \varphi$, difference between the intra/extra cellular potentials respectively. We use here the *modified monodomain* model (see [CLE 04]), $v(x, t)$ is given through a reaction diffusion system involving a second variable $\mathbf{w}(x, t) \in \mathbb{R}^N$ that describes the cells membrane activity (N is up to 20). It is used to simulate the normal propagation of excitation potential wave fronts (v passing from a rest value to a plateau value) and de-excitation, see figure 3. It reads :

$$A_m C_m \frac{\partial v}{\partial t} + A_m I_{ion}(v, \mathbf{w}) = \text{div}(G_1 \nabla v) + I_{app}(x, t), \quad \frac{\partial \mathbf{m}}{\partial t} = g(v, \mathbf{w}). \quad (8)$$

A_m, C_m are constants, G_1 is a non constant anisotropy tensor described below, I_{ion} , g are reaction terms and I_{app} a source term (applied current) that activates the system. The electrocardiograms (ECG) is the body surface potential resulting from that cardiac electrical activity. It is the trace on the torso T boundary ∂T of the extracellular potential φ . In the extra cardiac $T - H$, $\varphi(x, t)$ is given by a Poisson equation $\text{div}(G_T \nabla \varphi) = 0$, where G_T is isotropic heterogeneous between the different tissue layers conductivities (lungs, blood...). In the heart H , current balance between the intra and extra cellular compartments gives $\text{div}(G_2 \nabla \varphi) = -\text{div}(G_3 \nabla v)$. The tensors

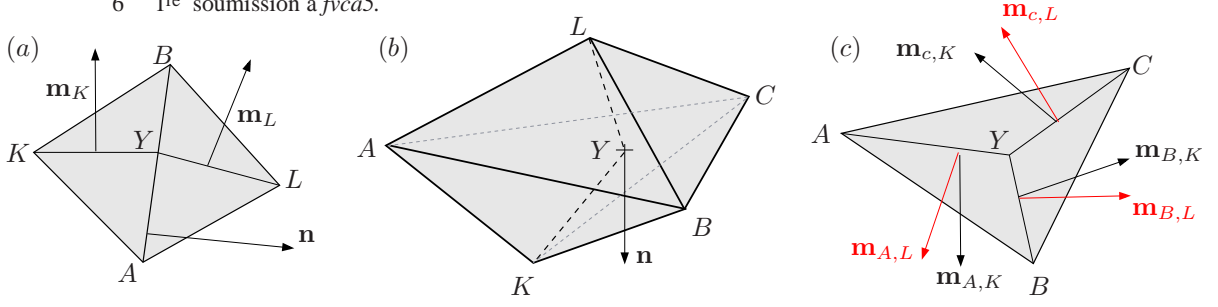


Figure 3. Notations for the gradient definition. (a) Two dimensional case : interface $\sigma = AB = C_K|C_L$ of centre Y , the three vectors \mathbf{n} , \mathbf{m}_K , \mathbf{m}_L have unit length and are respectively orthogonal to σ , YK , YL . Three dimensional case. (b) Interface $\sigma = ABC = C_K|C_L$ of centre Y , \mathbf{n} its unit normal from C_K towards C_L . (c) Same interface σ view from above, all vectors have unit length, $\mathbf{m}_{A,K}$, $\mathbf{m}_{B,K}$ and $\mathbf{m}_{C,K}$ are orthogonal to AYK , BYK and CYK respectively; same thing for $\mathbf{m}_{A,L}$, $\mathbf{m}_{B,L}$ and $\mathbf{m}_{C,L}$ by turning K into L .

G_i take into account the fibrous organisation of the heart. They read the same anisotropic/non constant form : $G_i(x) = P^{-1}(x)\tilde{G}_iP(x)$, where $\tilde{G}_i = \text{Diag}(g_i^l, g_i^t)$ is a reference matrix : g_i^l, g_i^t being the longitudinal/transverse conductivities along/across the cardiac fibres. $P(x)$ then is a change of basis matrix from the Frenet basis attached to the fibre direction at point x . On the whole domain T , this results in one global elliptic equation per time instant t :

$$\text{div}(G\nabla\varphi(t)) = f(v(t)) , \quad f(v(t)) = \begin{cases} 0 & \text{in } H \\ -\text{div}(G_3\nabla v(t)) & \text{in } T - H \end{cases} , \quad (9)$$

completed with the transmission conditions (2) on the heart/torso boundary and also on the interface between different tissue layers, and also with a Neumann boundary condition on ∂T (no current flow out of the body). In that problem, $v(x, t)$ is an entry coming from a first computation on the heart previously described.

We then discretised (9) using the DDFV scheme. Our domain T is a torso slice mesh coming from MRI segmented data and counting 600 000 degrees of freedom. The domain is divided in four parts : the heart, the ventricles cavities (filled in with blood), the lungs and the remaining torso. each part having the different previously described conductivity properties. φ is computed on T at each ms , the ECG body surface potential is recorded at 6 leads located on the torso boundary, see figure 3. On a whole cardiac cycle ($\simeq 600 ms$), 600 computation are thus performed. That computation necessitates the inversion of an ill-conditioned symmetric positive linear system at each ms . For this a Gm-Res solver combined with a basic SSOR preconditioning has been used.

A. Discrete gradient implementation

With the notations of *def.* 2.1 and of figure A, the expression of $\nabla_h \varphi_h$ is :

$$\begin{aligned} d = 2 : \quad 2D_{\sigma,K} (\nabla_h \varphi_h)_{\sigma,K} &= (\tilde{\varphi}(Y) - \varphi_K) \sigma \mathbf{n} + (\varphi_B - \varphi_A) KY \mathbf{m}_K \\ d = 3 : \quad 3D_{\sigma,K} (\nabla_h \varphi_h)_{\sigma,K} &= (\tilde{\varphi}(Y) - \varphi_K) \sigma \mathbf{n} + (\varphi_B - \varphi_C) AY K \mathbf{m}_{A,K} \\ &\quad + (\varphi_C - \varphi_A) BY K \mathbf{m}_{B,K} + (\varphi_A - \varphi_B) CY K \mathbf{m}_{C,K} \end{aligned}$$

It involves the DDFV function $\tilde{\varphi}_h$ in *def.* 2.1, whose definition is completed by :

$$\begin{aligned} d = 2 : \quad \tilde{\varphi}_h(Y) &= \alpha \varphi_K + (1 - \alpha) \varphi_L + k(\varphi_B - \varphi_A) \\ d = 3 : \quad \tilde{\varphi}_h(Y) &= \alpha \varphi_K + (1 - \alpha) \varphi_L + k_A(\varphi_B - \varphi_C) + k_B(\varphi_C - \varphi_A) + k_C(\varphi_A - \varphi_B) . \end{aligned}$$

with :

$$\begin{aligned} \alpha^{-1} &= 1 + \frac{D_{\sigma,K}}{D_{\sigma,L}} \frac{\mathbf{n} G_{\sigma,L} \mathbf{n}}{\mathbf{n} G_{\sigma,K} \mathbf{n}} \\ k &= \frac{LY}{\sigma} \frac{\mathbf{m}_L G_{\sigma,L} \mathbf{n}}{\frac{D_{\sigma,L}}{D_{\sigma,K}} \mathbf{n} G_{\sigma,K} \mathbf{n} + \mathbf{n} G_{\sigma,L} \mathbf{n}} - \frac{KY}{\sigma} \frac{\mathbf{m}_K G_{\sigma,K} \mathbf{n}}{\frac{D_{\sigma,K}}{D_{\sigma,L}} \mathbf{n} G_{\sigma,L} \mathbf{n} + \mathbf{n} G_{\sigma,K} \mathbf{n}} \\ k_Z &= \frac{ZYL}{\sigma} \frac{\mathbf{m}_{Z,L} G_{\sigma,L} \mathbf{n}}{\frac{D_{\sigma,L}}{D_{\sigma,K}} \mathbf{n} G_{\sigma,K} \mathbf{n} + \mathbf{n} G_{\sigma,L} \mathbf{n}} - \frac{ZYK}{\sigma} \frac{\mathbf{m}_{Z,K} G_{\sigma,K} \mathbf{n}}{\frac{D_{\sigma,K}}{D_{\sigma,L}} \mathbf{n} G_{\sigma,L} \mathbf{n} + \mathbf{n} G_{\sigma,K} \mathbf{n}} , \quad Z = A, B, C. \end{aligned}$$

For boundary interfaces this expression is adapted as follows. For $\sigma \in \mathcal{I}^D$, $\tilde{\varphi}_h(Y) = 0$. For $\sigma \in \mathcal{I}^N$, one suppresses $D_{\sigma,L}$ by stating $L = Y$ and $G_{\sigma,L} = 0$.

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